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On the Generalized Langevin Equation for a Rouse Bead in a Nonequilibrium Bath

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Abstract We present the reduced dynamics of a bead in a Rouse chain which is submerged in a bath containing a driving agent that renders it out-of-equilibrium. We first review the generalized Langevin equation of the middle bead in an equilibrated bath. Thereafter, we introduce two driving forces. Firstly, we add a constant force that is applied to the first bead of the chain. We investigate how the generalized Langevin equation changes due to this perturbation for which the system evolves towards a steady state after some time. Secondly, we consider the case of stochastic active forces which will drive the system to a nonequilibrium state. Including these active forces results in an extra contribution to the second fluctuation-dissipation relation. The form of this active contribution is analysed for the specific case of Gaussian, exponentially correlated active forces. We also discuss the resulting rich dynamics of the middle bead in which various regimes of normal diffusion, subdiffusion and superdiffusion can be present.

Keywords Rouse model · Active processes · Nonequilibrium reduced dynamics

1 Introduction

Complex systems consisting of a very large number of constituents (e.g. colloidal particles suspended in a fluid) can, in principle, be deterministically described by Newton's laws of motion. Despite that, due to the enormous amount of degrees-of-freedom, the resulting set of equations will not be solvable, neither analytically nor numerically. However, one is often only interested in the dynamics of one, or a few, slow variables. We will refer to these variables as “the system”. One can think of the position of a tagged particle inside a bath of other smaller particles, or the evolution of a reaction coordinate used to describe the folding of a biopolymer. The equation of motion of the slow variable can then be obtained by integrating out the fast variables interacting with the slow one. This approach will produce a closed equation of motion for the slow variable [25]. Such an effective equation of motion is commonly known as a generalized Langevin equation. Within linear response, the generalized Langevin description introduces three distinct terms in the effective dynamics of the system: an effective potential, a non-Markovian friction force and a non-white effective noise. For a system in an equilibrium environment, the latter two are connected through the (second) fluctuation-dissipation relation.

The simplest example of a generalized Langevin equation is the original Langevin equation introduced by Paul Langevin in 1908 [6]. It gives the reduced dynamics of a Brownian particle in a fluid.

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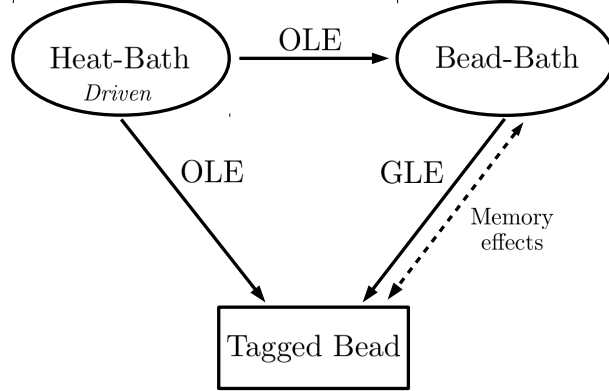


Fig. 1 Schematic representation of the applied description to acquire the reduced dynamics resulting from the different baths. OLE stands for original Langevin equation and GLE stands for generalized Langevin equation.

Equating the Newtonian inertial term are two forces, a Stokesian friction force and a thermal white noise. Both these forces are instantaneous, not influenced by the system’s past, implying that the original Langevin equation is a Markovian process for the position of the Brownian particle. This, rather simple, model is ideal to describe the diffusion of a small particle in a viscous fluid. That is because the time scale of collisions between the system and fluid particles, which correlates them, is very short.

The effective dynamics we will investigate, are those of a “tagged bead” in a Rouse chain. A Rouse chain is comprised of masses (or beads) linearly connected by harmonic springs and submerged in a viscous fluid. It is the simplest model for the dynamics of a polymer [3,14]. One of these beads will function as our system for which we construct its generalized Langevin equation. The dynamics of our system is influenced by two baths. First, we have the interaction with the particles of the fluid, which we refer to as the heat-bath. We apply the original Langevin equation to describe the reduced dynamics resulting from this bath. This implies that no memory effects will arise. Naturally, the heat-bath not only couples to the system but also to all other beads. Second, because the tagged bead is part of a chain, its dynamics depend on the evolution of the rest of the chain, which we call the bead-bath. Projecting the degrees-of-freedom of the bead-bath on the system will yield a generalized Langevin equation that represents the reduced dynamics of the system originating from the interaction with the chain. The bead-bath will therefore impose memory effects, which was to be expected due to the interconnected nature of the tagged bead and all other beads. Figure 1 gives a schematic representation on how the reduced dynamics of the tagged bead are acquired from the two baths.

For an equilibrated heat-bath the reduced dynamics of the tagged bead was already derived by D. Panja [11]. We will first give a short review of his findings. Our work extends these results to a heat-bath which is not in equilibrium but possesses some driving agent. We investigate two specific driving agents: a constant force on the first bead and nonconservative active forces.

A Rouse chain is widely known as a model that describes the dynamical properties of a polymer. A bead in the chain represents a rigid group of monomers. Several experiments study the diffusion of a tagged monomer when the polymer is surrounded by the complex cellular environment [2,24]. Knowing the effective dynamics of such a monomer is therefore crucial if one wants to interpret the observed diffusion, which often is anomalous. Furthermore, the cellular environment is certainly not in equilibrium. The nonequilibrium processes we study are therefore inspired by biological phenomena. The constant force on the first bead is a model for the process where molecular motors drag a polymer through the cellular environment in a well defined direction. This dragging takes, for example, place during cell division where the chromosomes are pulled apart by the mitotic spindle [12]. The active forces on the other hand model the overall non-thermal stress fluctuations inside cell, resulting from the action of molecular motors on the cytoskeleton. The precise characterisation of these active forces inside a cell or amidst *in vitro* cytoskeletons is a matter of current research [4,7,13]. We will assume the forces to be Gaussian as was recently shown to be true in artificial actin-myosin networks in a regime where the number of myosin motors is small [19]. Rouse chains subjected to active Gaussian

noise have been the focus of several recent papers [10,16,17,20], but so far the equation of motion of a tagged bead was not yet investigated.

2 From Rouse Model to Generalized Langevin Description

A Rouse chain is a simple model for a polymer devised by Prince E. Rouse in 1953 [14]. It comprises of N beads with mass m linearly connected by harmonic springs with spring constant k . This chain is submerged in a viscous heat-bath at temperature T and with friction coefficient γ . The motion of the n^{th} bead, with $n = 1, 2, \dots, N$, is given by the original Langevin equation. The position of this bead is given by vector $\mathbf{R}_n \in \mathbb{R}^3$, and thus we have

$$m \ddot{\mathbf{R}}_n(t) = -k \left(2\mathbf{R}_n(t) - \mathbf{R}_{n-1}(t) - \mathbf{R}_{n+1}(t) \right) - \gamma \dot{\mathbf{R}}_n(t) + \boldsymbol{\xi}_{T,n}(t). \quad (1)$$

In order to apply this formula to all beads, one introduces two ghost beads at $n = 0$ and $n = N+1$ whose positions satisfy $\mathbf{R}_0 = \mathbf{R}_1$ and $\mathbf{R}_{N+1} = \mathbf{R}_N$. The last two terms on the right-hand side of equation (1) represent the (reduced) interaction of the n^{th} bead with the heat-bath. They are, respectively, the Stokesian friction force and thermal agitation. These processes are connected through the fluctuation-dissipation relation which states that $\langle \boldsymbol{\xi}_{T,n}(t) \cdot \boldsymbol{\xi}_{T,m}(t') \rangle = 6\gamma k_B T \delta(t-t') \delta_{n,m}$, with k_B the Boltzmann constant. Furthermore, the thermal noise is assumed to be Gaussian with zero mean. The first term on the right-hand side originates from the harmonic interaction of the springs. If we assume to be in a low Reynolds number regime, we can apply the overdamped limit to this equation, i.e. $m/\gamma \ll 1$. This implies that the inertial term on the left-hand side of relation (1) is negligible and therefore drops out.

To acquire the reduced dynamics of a particular tagged bead, one can eliminate all other degrees-of-freedom from the set of equations of motion that expression (1) entails. This can be done by a change of variables to normal coordinates (see [3]). This effectively projects the dynamics of all beads on the dynamics of the tagged bead. It leads to an equation of motion known as the generalized Langevin equation of the system (i.e. the tagged bead). This calculation was first performed in [11] for the limit where n is taken as a continuous variable. We give the more general result of a discrete chain. The detailed derivation can be found in chapter 6 of [23]. A summary of the calculation is given in the appendix below. Here, we provide a short overview of the main results.

Consider a Rouse chain of $N = 2M + 1$ beads, the reduced dynamics of the position $\mathbf{r}(t) = \mathbf{R}_{M+1}(t)$ of the middle bead obeys the following generalized (overdamped) Langevin equation [11]

$$\gamma \dot{\mathbf{r}}(t) = \boldsymbol{\xi}_T(t) - \int_0^t d\tau K(t-\tau) \dot{\mathbf{r}}(\tau) + \boldsymbol{\Phi}(t). \quad (2)$$

The term on the left-hand side and the first term on the right-hand side of this equation are the viscous friction and thermal white noise acting on the middle bead, which already appeared in equation (1) and which have not been integrated out (they are, in fact, the projected variables of the heat-bath). The other two forces on the right-hand side of the equation of motion originate from the complex interaction with the remaining $2M$ beads. The convolution integral represents a non-Markovian friction on the middle bead. The past velocity profile of the bead influences the present friction, this influence is characterized by a memory kernel $K(t)$. The memory kernel is a large sum over decaying exponentials

$$K(t) = \frac{8k}{N} \sum_{p=1}^M \cos^2 \left(\frac{(2p-1)\pi}{2N} \right) \exp(-t/\tau_p). \quad (3)$$

The characteristic times of the exponentials are given by $\tau_p = \gamma N^2 / (k\pi^2(2p-1)^2)$ for large N . The slowest time $\tau_1 \sim N^2$ is referred to as the Rouse time and it is physically related to the time for the polymer to diffuse over its own radius of gyration. It can be shown that for large N this kernel has the following approximate form $K(t) \approx \sqrt{4\gamma k/\pi} \exp(-t/\tau_1) t^{-1/2}$, i.e. it displays an initial power-law decay followed by a decaying exponential. The last term in the equation of motion is the effective noise. An explicit expression of $\boldsymbol{\Phi}(t)$ is given in the appendix. Using that expression it can be shown that the effective noise is a Gaussian centered random variable whose correlation is connected to the non-Markovian friction through the fluctuation-dissipation relation. We have

$$\langle \boldsymbol{\Phi}(t) \cdot \boldsymbol{\Phi}(t') \rangle = 3k_B T K(|t-t'|). \quad (4)$$

From this equation it is clear that the effective noise is not white but correlated through time, i.e. it is coloured noise. Just as previous velocities of the system can influence its present friction, so will effective noise from the past have effect on the present effective noise. Both effects are dictated by the memory kernel. Because both noise terms, thermal and effective, obey the fluctuation-dissipation relation, the system will surely reach thermal equilibrium. Notice that in this case, the bead-bath does not produce an effective potential on the middle bead.

Two points need to be made about result (2). Firstly, as remarked in the introduction, a generalized Langevin equation for a slow variable is usually derived within linear response theory. As the Rouse model is linear, expression (2) is the full exact result. Secondly, the thermal noise $\xi_{T,n}(t)$ only contributes to $\Phi(t)$, not to the memory kernel $K(t)$. Mathematically this can be traced to $\xi_{T,n}(t)$ being a nonhomogeneous term in the set of equations (1). Adding other nonhomogeneous terms will therefore only lead to modifications of the noise-term of equation (2).

In the following two sections, we will assume that the heat-bath, in addition to the friction and thermal forces, also possesses some driving force that will pull our system away from equilibrium. First, we look at a constant force which is applied to the first bead. This force is conservative, but its potential does not have a minimum. Therefore, the system will not thermalize but rather arrive at a steady state after some characteristic time. The regime before the steady state, where the whole chain responds to the new force, is called the transient phase. Second, we assume the heat-bath exerts, apart from the thermal random forces, active random forces.

3 Constant Force

Applying a constant force to the first bead will add an extra term to equation (1). This term is given by $\mathbf{f}_n(t) = fH(t)\delta_{n,1}\mathbf{e}_x$. The strength of the force is determined by f and the Heaviside function $H(t)$ ensures that the force is turned on at $t = 0$. The arbitrary direction of the force is in the positive x -direction. The effect of such a term on the motion of a bead was already investigated by T. Sakaue [15]. We will however approach the problem from a slightly different angle.

Taking into account this force during the elimination of the bead-bath variables leads to the following reduced dynamics of the middle bead

$$\gamma \dot{\mathbf{r}}(t) = \xi_T(t) - \int_0^t d\tau K(t-\tau) \dot{\mathbf{r}}(\tau) + \Phi(t) + \mathcal{F}(t). \quad (5)$$

The new term on the right-hand side of this equation of motion represents the gradual increase of the constant force's influence on the middle bead. This effective force is given by (see [23] for the entire derivation)

$$\mathcal{F}(t) = \frac{2f}{N} \sum_{p=1}^M (-1)^p \cos\left(\frac{(2p-1)\pi}{2N}\right) \cot\left(\frac{(2p-1)\pi}{2N}\right) \left[\exp(-t/\tau_p) - 1\right] H(t) \mathbf{e}_x. \quad (6)$$

It is clear that when the elapsed time is much shorter than the smallest characteristic time, i.e. $t \ll \tau_M$, the effective force on the middle bead is essentially zero. The constant force has not yet had time to propagate through the chain to reach the middle bead, leaving this bead unaware of its presence. So for such early times we retrieve the equilibrium generalized Langevin equation (2), implying that the system remains thermalized. When the force does reach the tagged bead, the system will undergo a transient phase where the effective force on it will build up. We refer to [15] and [21], for a discussion on the resulting time-evolution of the system. For long times, $t \gg \tau_1$, the effective force takes on a constant value, causing the system to acquire a steady state velocity (see [21] for a discussion on this velocity). This constant value should be equal to the original applied force since it has fully propagated the chain. We indeed find this to be true for $N \gg 1$

$$\mathcal{F}(t \gg \tau_1) = -\frac{2f}{N} \sum_{p=1}^M (-1)^p \cos\left(\frac{(2p-1)\pi}{2N}\right) \cot\left(\frac{(2p-1)\pi}{2N}\right) \mathbf{e}_x = -\frac{2f}{N}(-M)\mathbf{e}_x = f \mathbf{e}_x. \quad (7)$$

Figure 2 shows the time-evolution of the effective force's magnitude compared to that of the constant force. It is a numerical evaluation of relation (6). As expected, the effective force is, for early times, zero

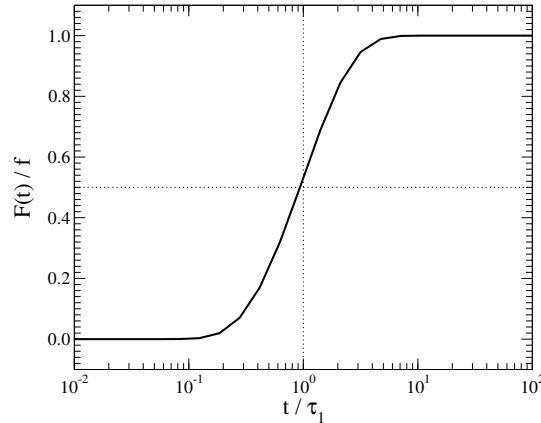


Fig. 2 Lin-log plot of the ratio of the effective force to the constant force as a function of time. We have $F(t) = |\mathcal{F}(t)|$. The vertical dotted line indicates the longest characteristic time τ_1 . The horizontal dotted line is drawn at $F/f = 1/2$. The number of beads is $N = 1025$, also $k_B T = \gamma = 1$ and $k = 3$, so $\tau_M/\tau_1 \approx 10^{-6}$.

and for long times it is equal to f . It reaches about half of its final value at the longest characteristic time τ_1 . In fact, in [21] it was shown that the effect of the force diffuses through the chain, so that the time to reach the middle bead is of the order $(N/2)^2$, i.e. this time is of the order of the Rouse time.

4 Active Forces

We now assume that in addition to thermal noise, the beads also feel active random forces. These could arise from the interaction of the polymer with active Brownian particles as was investigated in recent simulations [5, 18, 26]. Or they could represent active forces on a biopolymer immersed in a cell or in an artificial cytoskeleton [1]. To model this process, we add a stochastic term, $\xi_{A,n}(t)$, to the equations of motion (1). We first consider the general case where this new random force is Gaussian distributed with zero mean and a correlation that is a function of the absolute difference in time and uncorrelated between different beads

$$\langle \xi_{A,n}(t) \cdot \xi_{A,m}(t') \rangle = A(|t - t'|) \delta_{n,m} (1 - \delta_{n,M+1}). \quad (8)$$

The second delta assumes that the active random forces do not couple to the tagged bead. Extending the model to one where they do couple is trivial and does not yield conceptually different results. After eliminating the degrees-of-freedom of the chain, one finds that the expression of the generalized Langevin equation (2) still holds. There is no change in the friction term, the kernel $K(t)$ is still given by equation (3). The full expression for the noise $\Phi(t)$ in this case is again given in the appendix. It remains a centered Gaussian random variable. However, the correlation of the effective noise will be seriously affected. In a steady state regime, where t and t' are large, the correlation has the following expression

$$\langle \Phi(t) \cdot \Phi(t') \rangle_{neq} = 3k_B T \left(K(|t - t'|) + K_+(t, t') \right). \quad (9)$$

As can be seen, the correlation of the effective noise now comprises of two terms, the entropic memory kernel $K(t)$ from the equilibrium bath and a new memory kernel $K_+(t, t')$. At first sight, it may appear surprising that the active forces only modify the correlation of $\Phi(t)$. This is because the active forces in equation (1) do not couple to the dynamical variables $\mathbf{R}_n(t)$, they only appear as a nonhomogeneous term. If there would be a direct coupling between the active noise and the position of the beads, the former would also modify the kernel $K(t)$. From this expression we clearly see that the effective noise no longer obeys the fluctuation-dissipation relation, because no corresponding dissipative term exists for $K_+(t, t')$. Disobeying this relation results in a drift away from thermal equilibrium, hence the subscript “*neq*” which indicates the nonequilibrium character of this correlation. Result (9) is of the same form as that recently derived by C. Maes [8, 9] in a study of the second fluctuation-dissipation

relation out of equilibrium. In that work, $K_+(t, t')$ is referred to as the frenetic contribution and could be related to a change in dynamical activity of the fast variables. In our case, such an interpretation is not obvious to us. We therefore call $K_+(t, t')$ simply the “active contribution”. It is given by

$$K_+(t, t') = \frac{8k^2}{3\gamma^2 k_B T N} \sum_{p=1}^M \mathcal{S}_p^2 \int_0^t d\tau \int_0^{t'} d\tau' A(|\tau - \tau'|) \exp(-(t - \tau)/\tau_p) \exp(-(t' - \tau')/\tau_p), \quad (10)$$

where $\mathcal{S}_p = \sin((2p - 1)\pi/N)$.

The above expression for the active contribution can be solved for some specific forms of the correlation $A(t)$ of the new random force. Here we will present the case where the driving force is characterized by an exponential correlation because of its relevance for a polymer in a bath of active Brownian particles or in an actin-myosin network [7]. We assume

$$A(|t - t'|) = 3C \exp(-|t - t'|/\tau_A). \quad (11)$$

These active random forces can be understood as directionally persistent forces of characteristic strength \sqrt{C} and persistence time τ_A . This time gives the average time over which these random forces maintain their direction, after which they choose an uncorrelated new direction. After a lengthy, yet elementary, calculation one finds

$$K_+(|t - t'|) = \frac{8Ck^2}{\gamma^2 k_B T N} \sum_{p=1}^M \frac{\tau_p^2 \mathcal{S}_p^2}{1 - (\tau_p/\tau_A)^2} \left[\exp(-|t - t'|/\tau_A) - \left(\frac{\tau_p}{\tau_A} \right) \exp(-|t - t'|/\tau_p) \right]. \quad (12)$$

Just as the equilibrium memory kernel, the active contribution is a sum over exponentials and only a function of the absolute difference in time. It is possible to approximate this expression when we allow some assumptions on the active forces characteristics to be made.

4.1 Large persistence time

When $\tau_A \gg \tau_1$, we find the following simple form for the active contribution

$$K_+(|t - t'|) = \frac{CN}{k_B T} \exp(-|t - t'|/\tau_A). \quad (13)$$

We used here that $\sum_{p=1}^M (\tau_p \mathcal{S}_p)^2 = \gamma^2 N^2 / 8k^2$ for large N . This expression can be understood in the following way: in the previous section, on the constant force, we found that a force on a bead needs a duration of order τ_1 to fully reach the middle bead (see figure 2). Because the persistence in a particular direction of these active forces is indeed much longer than τ_1 , they act like a constant force for a considerable amount of time. Therefore, all beads fully transpose the active force on them to the middle bead, yielding N times equation (11). The nonequilibrium effective noise subsequently becomes

$$\langle \Phi(t) \cdot \Phi(t') \rangle_{neq} = 3k_B T K(|t - t'|) + NA(|t - t'|). \quad (14)$$

This result is general for any function $A(t)$ that decays with a typical time scale $\tau_A \gg \tau_1$. One can interpret this result as two effective noises. The first is the equilibrium thermal random force, governed by memory kernel $K(t)$. The second is the original active force that acts on every bead, but enhanced by a factor N .

4.2 Small persistence time

When we take $\tau_A \ll \tau_M$ in equation (12), we can do the following

$$K_+(|t - t'|) = -\frac{8Ck^2}{\gamma^2 k_B T N} \sum_{p=1}^M \tau_p^2 \mathcal{S}_p^2 \left[\exp(-|t - t'|/\tau_A) - \left(\frac{\tau_p}{\tau_A} \right) \exp(-|t - t'|/\tau_p) \right]. \quad (15)$$

Using the definition of the equilibrium memory kernel (3) and applying $\sum_{p=1}^M \mathcal{S}_p^2 \approx N/4$ for large N , results in

$$K_+(|t - t'|) = -\frac{2\tau_A^2 C k^2}{\gamma^2 k_B T} \exp(-|t - t'|/\tau_A) + \frac{\tau_A C}{\gamma k_B T} K(|t - t'|). \quad (16)$$

The first term in this expression can be neglected since the persistence time τ_A is very small. The nonequilibrium effective noise becomes

$$\langle \Phi(t) \cdot \Phi(t') \rangle_{neq} = 3k_B T_* K(|t - t'|), \quad (17)$$

with $k_B T_* = k_B T + \tau_A C/\gamma$. We thus find an effective noise that has an equilibrium expression but with a higher effective temperature than the case where no active forces are present. The system will therefore appear to thermalize under this new temperature. The reason for this behaviour is because the low-persistence-time active forces mimic the thermal noise $\xi_{T,n}(t)$ on the beads. Applying a well known representation of the Dirac delta function

$$\delta(x) = \lim_{\epsilon \rightarrow 0} \frac{1}{2\epsilon} \exp(-|x|/\epsilon), \quad (18)$$

the correlation of the active forces (i.e. equation (8) together with equation (11)) indeed becomes approximately equal to $6\tau_A C \delta(t - t') \delta_{n,m}$. The two Gaussian white noises, thermal and active, can thus be combined into one: $\xi_n(t) = \xi_{T,n}(t) + \xi_{A,n}(t)$. Naturally, this new random force is also Gaussian distributed with zero mean. Its correlation is

$$\langle \xi_n(t) \cdot \xi_m(t') \rangle = 6\gamma \left[k_B T + \frac{\tau_A C}{\gamma} \right] \delta(t - t') \delta_{n,m}. \quad (19)$$

When using this noise in equation (1) instead of $\xi_{T,n}(t)$, it is clear that we can redo the equilibrium calculations, but assuming the effective temperature T_* . This will also yield the nonequilibrium effective noise (17) derived above.

Figure 3 shows the numerical evaluation of $K(t)$ and $K_+(t)$, equations (3) and (12) respectively. For very early times, the equilibrium memory kernel is constant. Thereafter, for times up to τ_1 , this kernel shows a power-law decay after which it crosses over to an exponential decay, as was mentioned before. The behaviour of the active contribution $K_+(t)$ correctly shows a dependency on the value of τ_A . In the left of figures 4 we demonstrate that for small persistence time τ_A , the active contribution is indeed equal to the equilibrium memory kernel multiplied by $\tau_A C/\gamma k_B T$. For large persistence time τ_A on the other hand, the right of figures 4 shows that $K(t)$ is not exponential for early times while $K_+(t)$ is for all times, corresponding nicely with equation (13). The maximum value of the active contribution $K_+(t)$ never exceeds $CN/k_B T$, which figure 3 clearly shows.

5 Resulting motion of the tagged bead

To find the time-evolution of the middle bead, one should solve equation (2) using the nonequilibrium version of the fluctuation-dissipation relation (9). Since the equation is linear, this can easily be done using Laplace transform methods. Alternatively, one could solve the set of equations of motion (1) with the inclusion of active forces. This alternative derivation was already performed in [20]. In that paper, the more general case of a Rouse chain moving in a viscoelastic environment and in the presence of active forces was studied. Little attention was paid to the viscous limit.

Using the results of [20] or by direct solution of equation (2) it is possible to obtain the mean squared displacement $\Delta^2(t) \equiv \langle (\mathbf{r}(t) - \mathbf{r}(0))^2 \rangle$ of the middle bead for the case of exponentially correlated active noise. The result, with $\tilde{\tau}_p = \tau_{(p+1)/2}$, is given by

$$\begin{aligned} \Delta^2(t) = & \frac{6}{\gamma N} \left(k_B T + \frac{\tau_A C}{\gamma} \right) t + \frac{12 k_B T}{\gamma N} \sum_{p=2, \text{even}}^{N-1} \tilde{\tau}_p \left(1 - \exp(-t/\tilde{\tau}_p) \right) + \frac{6 \tau_A^2 C}{\gamma^2 N} \left(\exp(-t/\tau_A) - 1 \right) \\ & + \frac{12 C}{\gamma^2 N} \sum_{p=2, \text{even}}^{N-1} \frac{\tau_A \tilde{\tau}_p^2}{\tau_A - \tilde{\tau}_p} \left[\frac{\tau_A}{\tau_A + \tilde{\tau}_p} \left(1 - \exp(-(\tau_A^{-1} + \tilde{\tau}_p^{-1})t) \right) + \frac{1}{2} \left(\exp(-2t/\tilde{\tau}_p) - 1 \right) \right]. \end{aligned} \quad (20)$$

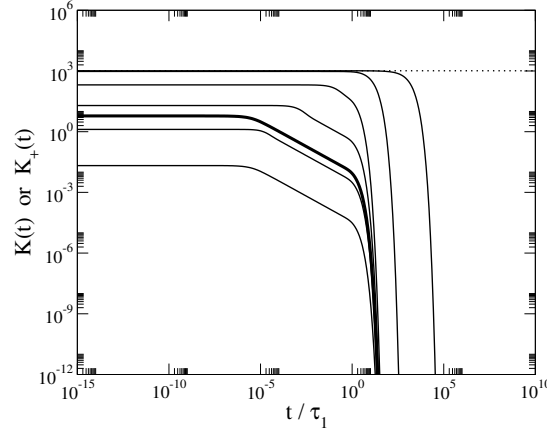


Fig. 3 Log-log plot of the two kernels as a function of time for $N = 1025$. The solid black line represents $K(t)$. The other thinner lines are $K_+(t)$ with $\tau_A/\tau_1 = 10^{-7}, 10^{-5}, 10^{-3}, 10^{-1}, 10^1$ and 10^3 . The higher the value of τ_A/τ_1 , the higher the line lies. The other parameters are $k_B T = \gamma = C = 1$ and $k = 3$. The straight dotted line is drawn at $CN/k_B T$.

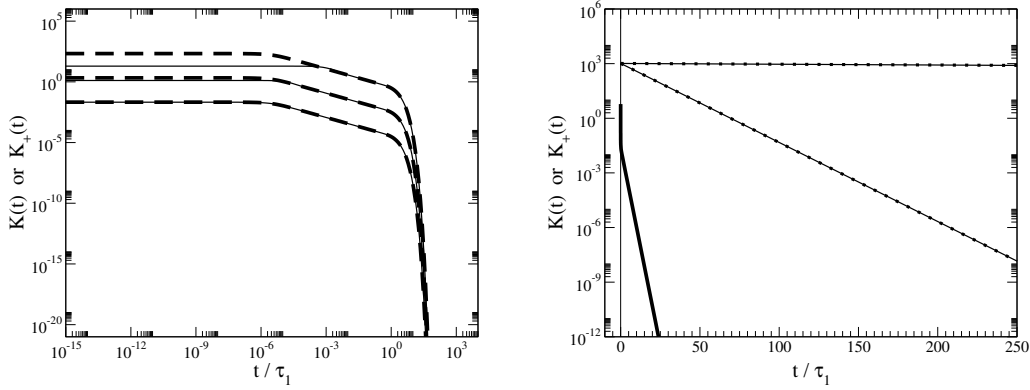


Fig. 4 Left: Log-log plot that shows the same three $K_+(t)$ curves from figure 3, with $\tau_A/\tau_1 = 10^{-7}, 10^{-5}$ and 10^{-3} . Also shown in dashed lines are the weighted equilibrium memory kernels, i.e. $(\tau_A C/\gamma k_B T)K(t)$. Right: Log-linear plot of the two upper $K_+(t)$ curves from figure 3, with $\tau_A/\tau_1 = 10^1$ and 10^3 . Also shown are $K(t)$ (solid black line) and equation (13) (dotted lines).

In absence of active forces ($C = 0$) only two terms survive. It is well known that for that case there are three time regimes [3,11]. For $t < \tau_M$, the bead doesn't feel the effect of the neighbouring beads yet, and it diffuses, i.e. $\Delta^2(t) \sim t$. For $t > \tau_1$ the bead follows the diffusion of the chain as a whole, i.e. we have again $\Delta^2(t) \sim t$ but with a diffusion constant that is a factor N smaller. Finally, in the intermediate time regime $\tau_M < t < \tau_1$ the bead feels that it is inside a chain leading to a subdiffusion with an exponent $1/2$, i.e. $\Delta^2(t) \sim t^{1/2}$. This behaviour is shown in Fig. 5 (dashed line).

In the presence of active forces the motion is more complicated. We first describe the motion of a free particle (i.e. a single bead, not constricted by springs) in presence of thermal and exponentially correlated active forces [22,23]. After a short initial period in which the particle shows normal diffusion, it will perform superdiffusion with an exponent 2, i.e. $\Delta^2(t) \sim t^2$, for the period in which the active forces are persistent, i.e. $t < \tau_A$. For $t > \tau_A$, the free particle will diffuse normally again.

We can now envisage two scenarios. First, consider the case of large persistence times, $\tau_A \gg \tau_1$. Analogous to the dynamics in absence of active forces, the bead will, for early and long times, behave as a free particle. However, in contrast to the non-active case, a free particle will display both diffusive and superdiffusive dynamics. So the bead will first diffuse, then cross-over to superdiffusion with $\Delta^2(t) \sim t^2$ and after that it will again diffuse. This behaviour is true for $t < \tau_M$ and $t > \tau_1$. For intermediate

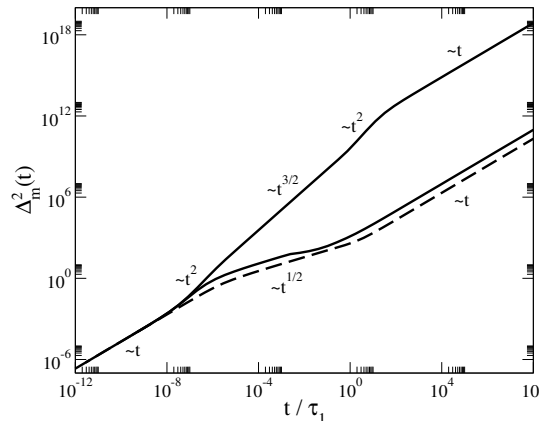


Fig. 5 Mean squared displacement of the middle bead in a Rouse chain in absence of active forces (dashed line) and in presence of active forces with small persistence time (lower full line, $\tau_A/\tau_1 = 10^{-7}$) and large persistence time (upper full line, $\tau_A/\tau_1 = 10$). Also indicated are the different regimes of diffusive, subdiffusive and superdiffusive behaviour.

times, however, the bead experiences the restriction of its neighbouring beads. This affects the superdiffusive regime and yields a superdiffusion with a smaller exponent. In [20], we derived that this exponent is equal to $3/2$. This type of behaviour indeed shows up if we plot $\Delta^2(t)$ as a function of time using expression (20) for $\tau_A = 10\tau_1$ (figure 5, upper full line). Second, we discuss the case of small persistence times, $\tau_A \ll \tau_M$. Now the bead will only show the behaviour of a free particle for times up to τ_A . So, after a short superdiffusive regime, the bead moves like a bead in a chain with only thermal noise, i.e. subdiffusion $\Delta^2(t) \sim t^{1/2}$ followed by diffusion with an amplitude that is N times smaller. However, this equilibrium-like behaviour has a somewhat larger prefactor. This is in agreement with what we learned in the previous section, where the behaviour of the bead could be described in terms of an effective temperature. This behaviour is shown in figure 5 (lower full line) for $\tau_A = 10^{-7}\tau_1$.

6 Conclusions

In the present paper, we studied the equation of motion of a bead in a Rouse chain with a constant force on the first bead and in an active environment. When the driving agent consisted of the constant force, we showed how this force propagates through the chain, increasing its influence on the middle bead. This introduced the middle bead to a transient phase after which it reached a steady state. When the active forces acted as the driving agent, we found that the fluctuation-dissipation relation picks up a new memory term. Apart from the equilibrium entropic memory kernel, an active contribution is added to the correlation of the effective noise. For exponentially correlated active forces, we found that when the persistence time is large, the active contribution is equal to N times the active correlation on a particular bead. When the persistence time is small, the system can be described with equilibrium reduced dynamics at an effective temperature $T_* = T + (\tau_A C / \gamma k_B T)$. These two regimes lead to two different possible motions for the tagged bead. For persistence times that are large in comparison with the Rouse time, various regions of diffusion and superdiffusion are expected. If, on the other hand, the persistence time is much smaller than the Rouse time, the only effect of the active forces will be that the motion in absence of active forces (diffusive to subdiffusive $\sim t^{1/2}$ to diffusive) is observed but the amplitude of that motion will be somewhat larger, an effect that can be seen as coming from the higher effective temperature.

Appendix

In this appendix we give a brief outline of our calculations. For more details we refer to chapter 6 of [23]. We consider a Rouse chain with $N = 2M + 1$ beads. Their position vectors obey the equation of motion (1). We will denote the position of the middle bead by $\mathbf{r}(t) = \mathbf{R}_{M+1}(t)$.

In order to derive the equation of motion for the middle bead, we introduce left and right normal coordinates $\mathbf{X}_p^L(t)$ and $\mathbf{X}_p^R(t)$ ($p = 1, 2, \dots, M$), which are defined as

$$\mathbf{X}_p^L(t) = \frac{2}{\sqrt{N}} \sum_{n=1}^M C_n^p \mathbf{R}_n(t), \quad (21)$$

$$\mathbf{X}_p^R(t) = -\frac{2}{\sqrt{N}} \sum_{n=M+2}^N C_n^p \mathbf{R}_n(t), \quad (22)$$

where the transformation coefficients C_n^p are given by

$$C_n^p = \cos\left(\frac{2p-1}{N} \left(n - \frac{1}{2}\right) \pi\right).$$

A long but straightforward calculation shows that these normal coordinates obey the following equations of motion

$$\gamma \dot{\mathbf{X}}_p^L(t) = -k\lambda_p \mathbf{X}_p^L(t) - (-1)^p \frac{2k}{\sqrt{N}} S_p \mathbf{r}(t) + \mathbf{f}_p^L(t), \quad (23)$$

$$\gamma \dot{\mathbf{X}}_p^R(t) = -k\lambda_p \mathbf{X}_p^R(t) - (-1)^p \frac{2k}{\sqrt{N}} S_p \mathbf{r}(t) + \mathbf{f}_p^R(t), \quad (24)$$

with $\lambda_p = 4 \sin^2((2p-1)\pi/2N)$, $S_p = \sin((2p-1)\pi/N)$ and

$$\mathbf{f}_p^L(t) = \frac{2}{\sqrt{N}} \sum_{n=1}^M C_n^p \boldsymbol{\xi}_{T,n}(t), \quad (25)$$

$$\mathbf{f}_p^R(t) = -\frac{2}{\sqrt{N}} \sum_{n=M+2}^N C_n^p \boldsymbol{\xi}_{T,n}(t). \quad (26)$$

The differential equations (23-24) are uncoupled, linear and nonhomogeneous. They can therefore be solved immediately. Inverting (21-22), we can write the positions of the beads in terms of the normal coordinates. This gives (for $n = 1, 2, \dots, M$ and $m = M+2, M+3, \dots, N$)

$$\mathbf{R}_n(t) = \frac{2}{\sqrt{N}} \sum_{p=1}^M C_n^p \mathbf{X}_p^L(t), \quad (27)$$

$$\mathbf{R}_m(t) = -\frac{2}{\sqrt{N}} \sum_{p=1}^M C_m^p \mathbf{X}_p^R(t). \quad (28)$$

Using these expressions one can easily show that the position of the middle bead evolves according to

$$\gamma \dot{\mathbf{r}}(t) = \boldsymbol{\xi}_T(t) - 2k\mathbf{r}(t) - \frac{2k}{\sqrt{N}} \sum_{p=1}^M (-1)^p S_p \left(\mathbf{X}_p^L(t) + \mathbf{X}_p^R(t) \right). \quad (29)$$

Inserting the solutions of (23-24) gives for the equation of motion of the tagged middle bead

$$\begin{aligned} \gamma \dot{\mathbf{r}}(t) = & \boldsymbol{\xi}_T(t) - 2k\mathbf{r}(t) - \frac{2k}{\sqrt{N}} \sum_{p=1}^M (-1)^p S_p \left[\left(\mathbf{X}_p^L(0) + \mathbf{X}_p^R(0) \right) e^{-t/\tau_p} \right. \\ & \left. + \frac{1}{\gamma} \int_0^t d\tau \left(\mathbf{f}_p^L(\tau) + \mathbf{f}_p^R(\tau) \right) e^{(\tau-t)/\tau_p} - (-1)^p \frac{4k}{\gamma\sqrt{N}} S_p \int_0^t d\tau \mathbf{r}(\tau) e^{(\tau-t)/\tau_p} \right]. \end{aligned} \quad (30)$$

The last integral can be rewritten using integration by parts

$$\int_0^t d\tau \mathbf{r}(\tau) e^{(\tau-t)/\tau_p} = \tau_p \mathbf{r}(t) - \tau_p \mathbf{r}(0) e^{-t/\tau_p} - \tau_p \int_0^t d\tau e^{(\tau-t)/\tau_p} \dot{\mathbf{r}}(\tau).$$

When we put this back into the equation of motion, we can group some terms and identify them in the context of the generalized Langevin equation. We finally get

$$\gamma \dot{\mathbf{r}}(t) = \boldsymbol{\xi}_T(t) - \int_0^t d\tau K(t-\tau) \dot{\mathbf{r}}(\tau) + \boldsymbol{\Phi}(t), \quad (31)$$

where the memory kernel equals

$$K(t) = \frac{8k^2}{\gamma N} \sum_{p=1}^M \tau_p S_p^2 e^{-t/\tau_p}, \quad (32)$$

and the effective noise is given by

$$\begin{aligned} \boldsymbol{\Phi}(t) = -\frac{2k}{\sqrt{N}} \sum_{p=1}^N (-1)^p S_p e^{-t/\tau_p} \left[\mathbf{X}_p^L(0) + \mathbf{X}_p^R(0) + (-1)^p \frac{4k}{\sqrt{N}} \tau_p S_p \mathbf{r}(0) \right. \\ \left. + \frac{1}{\gamma} \int_0^t d\tau \left(\mathbf{f}_p^L(\tau) + \mathbf{f}_p^R(\tau) \right) e^{\tau/\tau_p} \right]. \end{aligned} \quad (33)$$

From this definition and the relations (25-26), it can be seen $\boldsymbol{\Phi}(t)$ is a Gaussian random variable. Long yet straightforward calculations can show that the average of this random variable is zero and that its correlation is given by relation (4).

When active forces $\boldsymbol{\xi}_{A,n}(t)$ are added, the calculation proceeds along the same line. The main difference is that the functions $\mathbf{f}_p^L(t)$ and $\mathbf{f}_p^R(t)$ are modified to include the active forces. The definitions (25-26) are now replaced by

$$\mathbf{f}_p^L(t) = \frac{2}{\sqrt{N}} \sum_{n=1}^M C_n^p \left(\boldsymbol{\xi}_{T,n}(t) + \boldsymbol{\xi}_{A,n}(t) \right), \quad (34)$$

$$\mathbf{f}_p^R(t) = -\frac{2}{\sqrt{N}} \sum_{n=M+2}^N C_n^p \left(\boldsymbol{\xi}_{T,n}(t) + \boldsymbol{\xi}_{A,n}(t) \right). \quad (35)$$

With this modified definition, the equations of motion of the normal coordinates are still given by (23-24) and the equation of motion of the tagged particles is still given by (30). As a result the memory kernel $K(t)$ is not modified. The only difference is that the extra terms due to the active forces in (34-35) will lead to a different form for the effective noise correlation. Another calculation then leads to the results for the noise correlation given in the main text, i.e. the expressions (9) and (10).

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